



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 7, 2020 – 11:31 am BST

PDB ID : 6TPJ
Title : Crystal structure of the Orexin-2 receptor in complex with suvorexant at 2.76 Å resolution
Authors : Rappas, M.; Ali, A.; Bennett, K.A.; Brown, J.D.; Bucknell, S.J.; Congreve, M.; Cooke, R.M.; Cseke, G.; de Graaf, C.; Dore, A.S.; Errey, J.C.; Jazayeri, A.; Marshall, F.H.; Mason, J.S.; Mould, R.; Patel, J.C.; Tehan, B.G.; Weir, M.; Christopher, J.A.
Deposited on : 2019-12-13
Resolution : 2.74 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

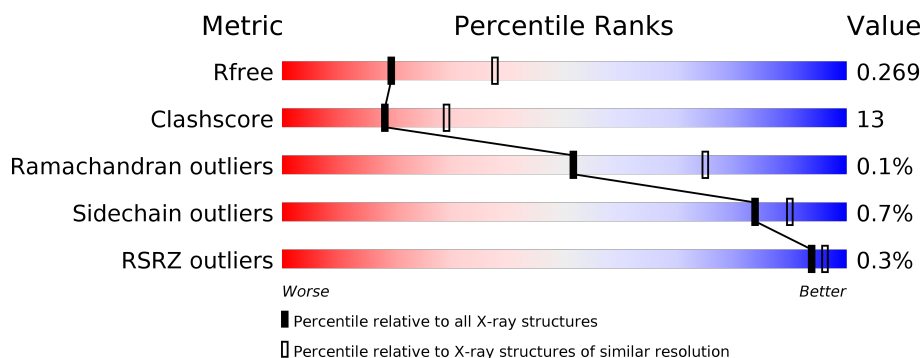
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	564	 70% 18% • 12%
1	B	564	 66% 22% • 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8644 atoms, of which 66 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Orexin receptor type 2, GlgA glycogen synthase, Hypocretin receptor-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			3979	2612	659	678	30			
1	B	501	Total	C	N	O	S	0	0	0
			4000	2624	664	682	30			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLN	-	expression tag	UNP O43614
A	-9	ASP	-	expression tag	UNP O43614
A	-8	LEU	-	expression tag	UNP O43614
A	-7	ASP	-	expression tag	UNP O43614
A	-6	TYR	-	expression tag	UNP O43614
A	-5	LYS	-	expression tag	UNP O43614
A	-4	ASP	-	expression tag	UNP O43614
A	-3	ASP	-	expression tag	UNP O43614
A	-2	ASP	-	expression tag	UNP O43614
A	-1	ASP	-	expression tag	UNP O43614
A	0	LYS	-	expression tag	UNP O43614
A	14	ASP	ASN	engineered mutation	UNP O43614
A	22	ASP	ASN	engineered mutation	UNP O43614
A	28	LEU	PHE	engineered mutation	UNP O43614
A	30	ASP	ASN	engineered mutation	UNP O43614
A	54	ALA	GLU	engineered mutation	UNP O43614
A	91	LEU	TYR	engineered mutation	UNP O43614
A	100	ALA	ASP	engineered mutation	UNP O43614
A	142	ALA	VAL	engineered mutation	UNP O43614
A	170	LEU	ARG	engineered mutation	UNP O43614
A	202	ASP	ASN	engineered mutation	UNP O43614
A	206	ALA	LEU	engineered mutation	UNP O43614
A	219	ALA	TYR	engineered mutation	UNP O43614
A	233	ALA	MET	engineered mutation	UNP O43614

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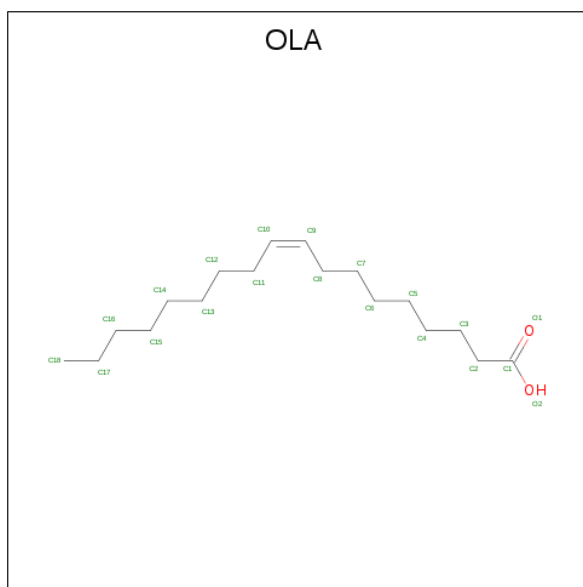
Chain	Residue	Modelled	Actual	Comment	Reference
A	242	LEU	ALA	engineered mutation	UNP O43614
A	310	VAL	LEU	engineered mutation	UNP Q548Y0
A	318	ALA	LEU	engineered mutation	UNP Q548Y0
A	347	ALA	THR	engineered mutation	UNP Q548Y0
A	381	TRP	CYS	engineered mutation	UNP Q548Y0
A	382	TRP	CYS	engineered mutation	UNP Q548Y0
A	383	TRP	CYS	engineered mutation	UNP Q548Y0
A	389	HIS	-	expression tag	UNP Q548Y0
A	390	HIS	-	expression tag	UNP Q548Y0
A	391	HIS	-	expression tag	UNP Q548Y0
A	392	HIS	-	expression tag	UNP Q548Y0
A	393	HIS	-	expression tag	UNP Q548Y0
A	394	HIS	-	expression tag	UNP Q548Y0
A	395	HIS	-	expression tag	UNP Q548Y0
A	396	HIS	-	expression tag	UNP Q548Y0
B	-10	GLN	-	expression tag	UNP O43614
B	-9	ASP	-	expression tag	UNP O43614
B	-8	LEU	-	expression tag	UNP O43614
B	-7	ASP	-	expression tag	UNP O43614
B	-6	TYR	-	expression tag	UNP O43614
B	-5	LYS	-	expression tag	UNP O43614
B	-4	ASP	-	expression tag	UNP O43614
B	-3	ASP	-	expression tag	UNP O43614
B	-2	ASP	-	expression tag	UNP O43614
B	-1	ASP	-	expression tag	UNP O43614
B	0	LYS	-	expression tag	UNP O43614
B	14	ASP	ASN	engineered mutation	UNP O43614
B	22	ASP	ASN	engineered mutation	UNP O43614
B	28	LEU	PHE	engineered mutation	UNP O43614
B	30	ASP	ASN	engineered mutation	UNP O43614
B	54	ALA	GLU	engineered mutation	UNP O43614
B	91	LEU	TYR	engineered mutation	UNP O43614
B	100	ALA	ASP	engineered mutation	UNP O43614
B	142	ALA	VAL	engineered mutation	UNP O43614
B	170	LEU	ARG	engineered mutation	UNP O43614
B	202	ASP	ASN	engineered mutation	UNP O43614
B	206	ALA	LEU	engineered mutation	UNP O43614
B	219	ALA	TYR	engineered mutation	UNP O43614
B	233	ALA	MET	engineered mutation	UNP O43614
B	242	LEU	ALA	engineered mutation	UNP O43614
B	310	VAL	LEU	engineered mutation	UNP Q548Y0
B	318	ALA	LEU	engineered mutation	UNP Q548Y0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	347	ALA	THR	engineered mutation	UNP Q548Y0
B	381	TRP	CYS	engineered mutation	UNP Q548Y0
B	382	TRP	CYS	engineered mutation	UNP Q548Y0
B	383	TRP	CYS	engineered mutation	UNP Q548Y0
B	389	HIS	-	expression tag	UNP Q548Y0
B	390	HIS	-	expression tag	UNP Q548Y0
B	391	HIS	-	expression tag	UNP Q548Y0
B	392	HIS	-	expression tag	UNP Q548Y0
B	393	HIS	-	expression tag	UNP Q548Y0
B	394	HIS	-	expression tag	UNP Q548Y0
B	395	HIS	-	expression tag	UNP Q548Y0
B	396	HIS	-	expression tag	UNP Q548Y0

- Molecule 2 is OLEIC ACID (three-letter code: OLA) (formula: C₁₈H₃₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	A	1	Total	C	O	0	0
			11	9	2		
2	A	1	Total	C	O	0	0
			7	5	2		
2	A	1	Total	C		0	0
			6	6			
2	A	1	Total	C	O	0	0
			9	7	2		

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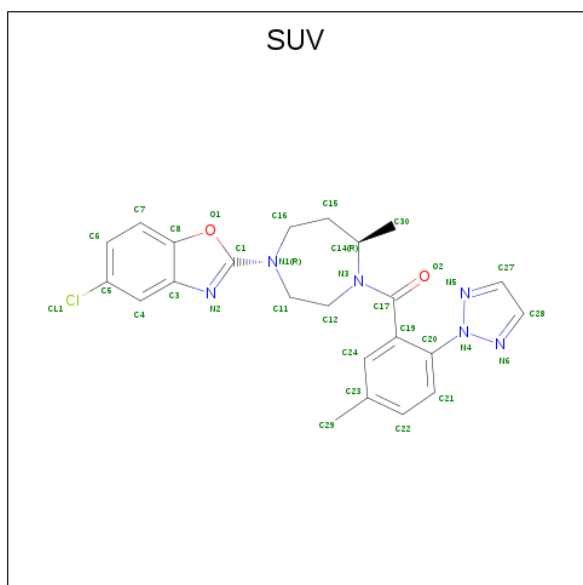
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 8 6 2	0	0
2	A	1	Total C O 11 9 2	0	0
2	A	1	Total C 6 6	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C 15 15	0	0
2	A	1	Total C O 14 12 2	0	0
2	A	1	Total C O 6 4 2	0	0
2	A	1	Total C 6 6	0	0
2	B	1	Total C O 6 4 2	0	0
2	B	1	Total C O 7 5 2	0	0
2	B	1	Total C 5 5	0	0
2	B	1	Total C O 9 7 2	0	0
2	B	1	Total C O 6 4 2	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C O 20 18 2	0	0
2	B	1	Total C O 7 5 2	0	0
2	B	1	Total C 5 5	0	0
2	B	1	Total C O 7 5 2	0	0
2	B	1	Total C 4 4	0	0
2	B	1	Total C 5 5	0	0
2	B	1	Total C 7 7	0	0

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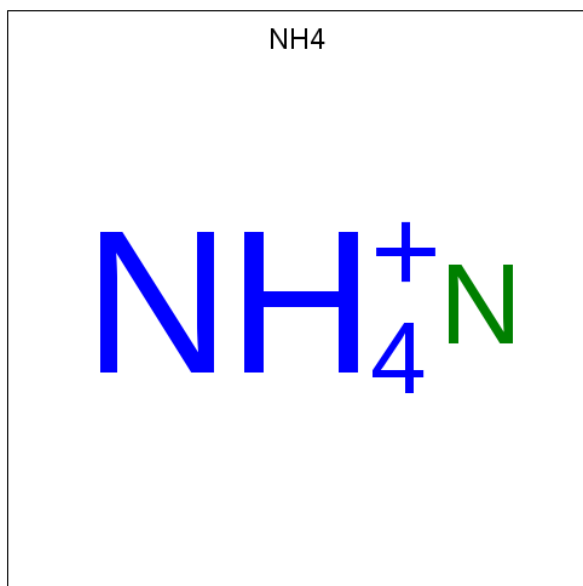
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			17	15	2		
2	B	1	Total	C	O	0	0
			10	8	2		
2	B	1	Total	C	O	0	0
			8	6	2		
2	B	1	Total	C	O	0	0
			8	6	2		
2	B	1	Total	C		0	0
			7	7			
2	B	1	Total	C		0	0
			6	6			
2	B	1	Total	C		0	0
			5	5			
2	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is [(7R)-4-(5-chloro-1,3-benzoxazol-2-yl)-7-methyl-1,4-diazepan-1-yl][5-methyl-2-(2H-1,2,3-triazol-2-yl)phenyl]methanone (three-letter code: SUV) (formula: C₂₃H₂₃ClN₆O₂) (labeled as "Ligand of Interest" by author).



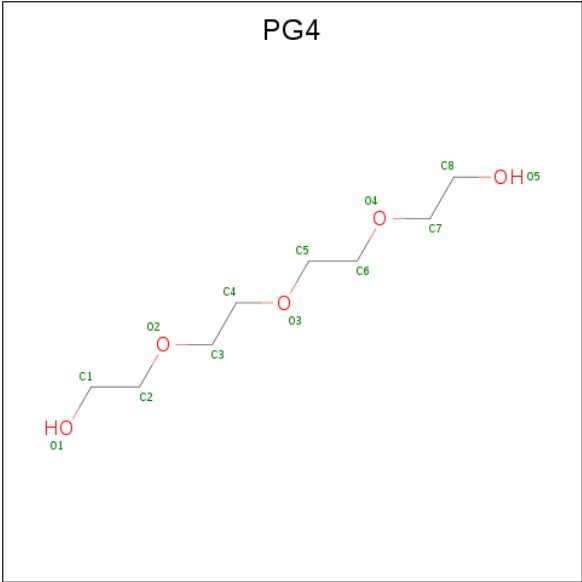
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	H	N	O	0	0
			55	23	1	23	6	2		
3	B	1	Total	C	Cl	H	N	O	0	0
			55	23	1	23	6	2		

- Molecule 4 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	H	N	0	0
			5	4	1		
4	A	1	Total	H	N	0	0
			5	4	1		
4	B	1	Total	H	N	0	0
			5	4	1		
4	B	1	Total	H	N	0	0
			5	4	1		
4	B	1	Total	H	N	0	0
			5	4	1		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $\text{C}_8\text{H}_{18}\text{O}_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		
5	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	114	Total	O	0	0
			114	114		
6	B	112	Total	O	0	0
			112	112		

E1186	M1187	K1190	M1193	S1196	K294	R297	Y308	Y312	C316	Y317	A318	F319	N324	K327	R332	R339	N360	P361	N365	F375	K376	S380	N381	N382	N383	L384	G385	N386	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS
-------	-------	-------	-------	-------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.33Å 76.25Å 82.74Å 89.99° 85.25° 89.97°	Depositor
Resolution (Å)	47.70 – 2.74 47.69 – 2.73	Depositor EDS
% Data completeness (in resolution range)	67.2 (47.70-2.74) 81.4 (47.69-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.59 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.207 , 0.254 0.235 , 0.269	Depositor DCC
R_{free} test set	1634 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 17.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.437 for -h,k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8644	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OLA, NH4, PG4, YCM, SUV

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.37	1/4066 (0.0%)	0.64	1/5509 (0.0%)
1	B	0.36	0/4088	0.67	4/5540 (0.1%)
All	All	0.37	1/8154 (0.0%)	0.65	5/11049 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1137	ILE	C-N	8.49	1.50	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1102	ARG	NE-CZ-NH1	-10.76	114.92	120.30
1	A	297	ARG	NE-CZ-NH1	-10.29	115.15	120.30
1	B	297	ARG	NE-CZ-NH2	-8.39	116.10	120.30
1	B	1102	ARG	NE-CZ-NH2	7.96	124.28	120.30
1	B	297	ARG	NE-CZ-NH1	5.36	122.98	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1136	ALA	Mainchain
1	B	52	GLU	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3979	0	4073	100	0
1	B	4000	0	4097	126	0
2	A	114	0	147	17	0
2	B	164	0	219	26	0
3	A	32	23	23	3	0
3	B	32	23	23	3	0
4	A	2	8	0	0	0
4	B	3	12	0	0	0
5	A	13	0	18	2	0
5	B	13	0	18	1	0
6	A	114	0	0	1	0
6	B	112	0	0	3	0
All	All	8578	66	8618	228	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 228 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:HIS:HB3	1:A:50:PRO:CD	1.65	1.22
1:A:49:HIS:CB	1:A:50:PRO:HD3	1.79	1.09
1:B:1009:GLU:HG2	1:B:1012:LEU:HD12	1.34	1.08
1:A:1137:ILE:HG21	1:A:1184:PHE:CE2	1.94	1.02
1:A:1137:ILE:HD13	1:A:1184:PHE:HD2	1.25	1.02

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	494/564 (88%)	483 (98%)	10 (2%)	1 (0%)	47	69
1	B	498/564 (88%)	485 (97%)	13 (3%)	0	100	100
All	All	992/1128 (88%)	968 (98%)	23 (2%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	HIS

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	428/491 (87%)	426 (100%)	2 (0%)	88	92
1	B	430/491 (88%)	426 (99%)	4 (1%)	78	87
All	All	858/982 (87%)	852 (99%)	6 (1%)	84	90

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	80	TRP
1	B	332	MET
1	B	167	LYS
1	A	1185	ARG
1	B	1184	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	YCM	B	147	1	7,9,10	0.58	0	4,10,12	0.55	0
1	YCM	A	147	1	7,9,10	0.59	0	4,10,12	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	YCM	B	147	1	-	4/6/8/10	-
1	YCM	A	147	1	-	4/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	147	YCM	N-CA-CB-SG
1	B	147	YCM	C-CA-CB-SG
1	B	147	YCM	SG-CD-CE-OZ1
1	B	147	YCM	SG-CD-CE-NZ2
1	A	147	YCM	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 43 ligands modelled in this entry, 5 are modelled with single atom - leaving 38 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	OLA	A	1207	-	5,5,19	0.23	0	4,4,19	0.40	0
2	OLA	B	2121	-	4,7,19	0.30	0	3,7,19	0.24	0
2	OLA	B	2125	-	4,7,19	0.33	0	3,7,19	0.29	0
2	OLA	A	1216	-	5,5,19	0.14	0	4,4,19	0.18	0
2	OLA	A	1211	-	5,5,19	0.12	0	4,4,19	0.11	0
5	PG4	A	1217	-	12,12,12	0.17	0	11,11,11	0.16	0
2	OLA	A	1215	-	2,5,19	0.23	0	2,5,19	0.51	0
2	OLA	A	1201	-	4,7,19	0.23	0	3,7,19	0.17	0
2	OLA	B	2124	-	4,4,19	0.15	0	3,3,19	0.23	0
5	PG4	B	2126	-	12,12,12	0.13	0	11,11,11	0.19	0
2	OLA	B	2116	-	4,4,19	0.13	0	3,3,19	0.21	0
2	OLA	A	1205	-	3,6,19	0.28	0	2,6,19	0.22	0
2	OLA	B	2117	-	6,6,19	0.14	0	5,5,19	0.08	0
2	OLA	B	2115	-	3,3,19	0.22	0	2,2,19	0.46	0
2	OLA	B	2118	-	13,16,19	0.25	0	12,16,19	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OLA	A	1214	-	10,13,19	0.23	0	8,13,19	0.23	0
2	OLA	B	2122	-	6,6,19	0.16	0	5,5,19	0.18	0
2	OLA	B	2119	-	6,9,19	0.35	0	5,9,19	0.30	0
2	OLA	A	1208	-	5,8,19	0.23	0	4,8,19	0.15	0
2	OLA	B	2120	-	4,7,19	0.25	0	3,7,19	0.21	0
2	OLA	B	2107	-	4,4,19	0.17	0	3,3,19	0.23	0
2	OLA	B	2110	-	6,6,19	0.15	0	5,5,19	0.14	0
2	OLA	B	2105	-	2,5,19	0.23	0	2,5,19	0.38	0
2	OLA	A	1210	1	7,10,19	0.17	0	6,10,19	0.14	0
2	OLA	A	1204	-	7,10,19	0.20	0	6,10,19	0.15	0
2	OLA	B	2109	-	2,5,19	0.23	0	2,5,19	0.43	0
2	OLA	A	1212	-	6,6,19	0.17	0	5,5,19	0.17	0
3	SUV	A	1202	-	31,36,36	0.93	1 (3%)	32,52,52	1.20	4 (12%)
2	OLA	A	1209	-	4,7,19	0.24	0	3,7,19	0.20	0
3	SUV	B	2101	-	31,36,36	0.97	2 (6%)	32,52,52	1.54	6 (18%)
2	OLA	B	2108	-	5,8,19	0.24	0	4,8,19	0.14	0
2	OLA	A	1213	-	14,14,19	0.21	0	13,13,19	0.15	0
2	OLA	B	2123	-	5,5,19	0.15	0	4,4,19	0.20	0
2	OLA	B	2113	-	4,4,19	0.13	0	3,3,19	0.22	0
2	OLA	B	2114	-	3,6,19	0.35	0	2,6,19	0.20	0
2	OLA	B	2111	-	16,19,19	0.25	0	15,19,19	0.12	0
2	OLA	B	2112	-	3,6,19	0.25	0	2,6,19	0.24	0
2	OLA	B	2106	-	3,6,19	0.27	0	2,6,19	0.24	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLA	A	1207	-	-	1/3/3/17	-
2	OLA	B	2121	-	-	1/3/5/17	-
2	OLA	B	2125	-	-	0/3/5/17	-
2	OLA	A	1216	-	-	0/3/3/17	-
2	OLA	A	1211	-	-	0/3/3/17	-
5	PG4	A	1217	-	-	3/10/10/10	-
2	OLA	A	1215	-	-	0/1/3/17	-
2	OLA	A	1201	-	-	2/3/5/17	-
2	OLA	B	2124	-	-	0/2/2/17	-
5	PG4	B	2126	-	-	2/10/10/10	-
2	OLA	B	2116	-	-	0/2/2/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLA	A	1205	-	-	0/2/4/17	-
2	OLA	B	2117	-	-	0/4/4/17	-
2	OLA	B	2115	-	-	0/1/1/17	-
2	OLA	B	2118	-	-	3/12/14/17	-
2	OLA	A	1214	-	-	2/9/11/17	-
2	OLA	B	2122	-	-	1/4/4/17	-
2	OLA	B	2119	-	-	2/5/7/17	-
2	OLA	A	1208	-	-	0/4/6/17	-
2	OLA	B	2120	-	-	0/3/5/17	-
2	OLA	B	2107	-	-	0/2/2/17	-
2	OLA	B	2110	-	-	0/4/4/17	-
2	OLA	B	2105	-	-	0/1/3/17	-
2	OLA	A	1210	1	-	1/6/8/17	-
2	OLA	A	1204	-	-	3/6/8/17	-
2	OLA	B	2109	-	-	0/1/3/17	-
2	OLA	A	1212	-	-	0/4/4/17	-
3	SUV	A	1202	-	-	2/10/30/30	0/4/5/5
2	OLA	A	1209	-	-	0/3/5/17	-
3	SUV	B	2101	-	-	2/10/30/30	0/4/5/5
2	OLA	B	2108	-	-	0/4/6/17	-
2	OLA	A	1213	-	-	3/12/12/17	-
2	OLA	B	2123	-	-	0/3/3/17	-
2	OLA	B	2113	-	-	0/2/2/17	-
2	OLA	B	2114	-	-	0/2/4/17	-
2	OLA	B	2111	-	-	1/15/17/17	-
2	OLA	B	2112	-	-	0/2/4/17	-
2	OLA	B	2106	-	-	0/2/4/17	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2101	SUV	C1-N2	-4.02	1.29	1.35
3	A	1202	SUV	C1-N2	-3.64	1.30	1.35
3	B	2101	SUV	C4-C3	-2.12	1.38	1.41

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2101	SUV	C15-C16-N1	-4.71	105.36	113.48
3	B	2101	SUV	C21-C20-C19	-4.06	119.25	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1202	SUV	C21-C20-C19	-3.81	119.48	122.95
3	B	2101	SUV	C30-C14-C15	3.20	117.67	111.74
3	A	1202	SUV	C15-C16-N1	-2.85	108.57	113.48

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

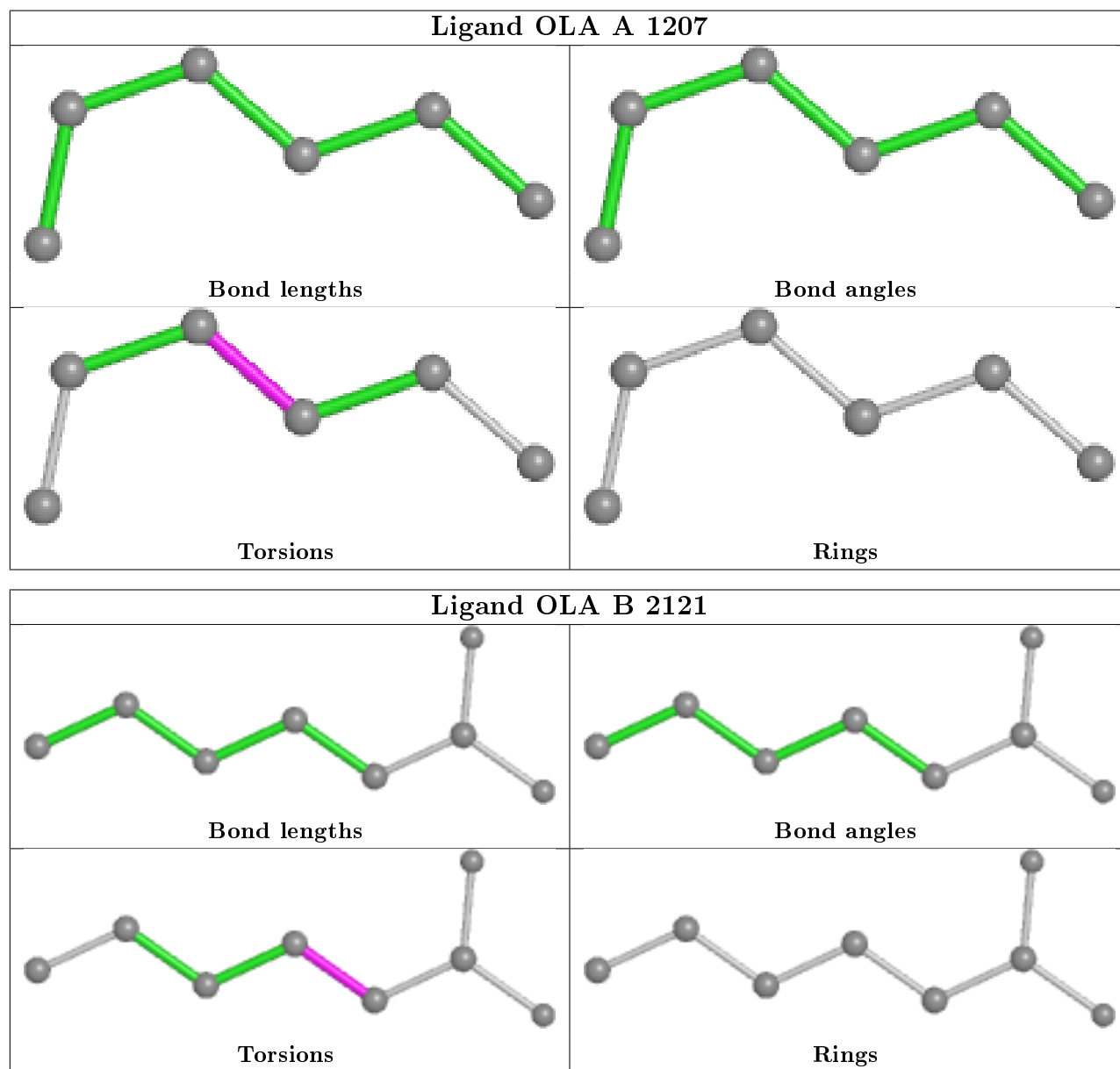
Mol	Chain	Res	Type	Atoms
2	A	1201	OLA	C1-C2-C3-C4
2	A	1210	OLA	C1-C2-C3-C4
2	A	1204	OLA	C1-C2-C3-C4
3	A	1202	SUV	C21-C20-N4-N5
3	A	1202	SUV	C21-C20-N4-N6

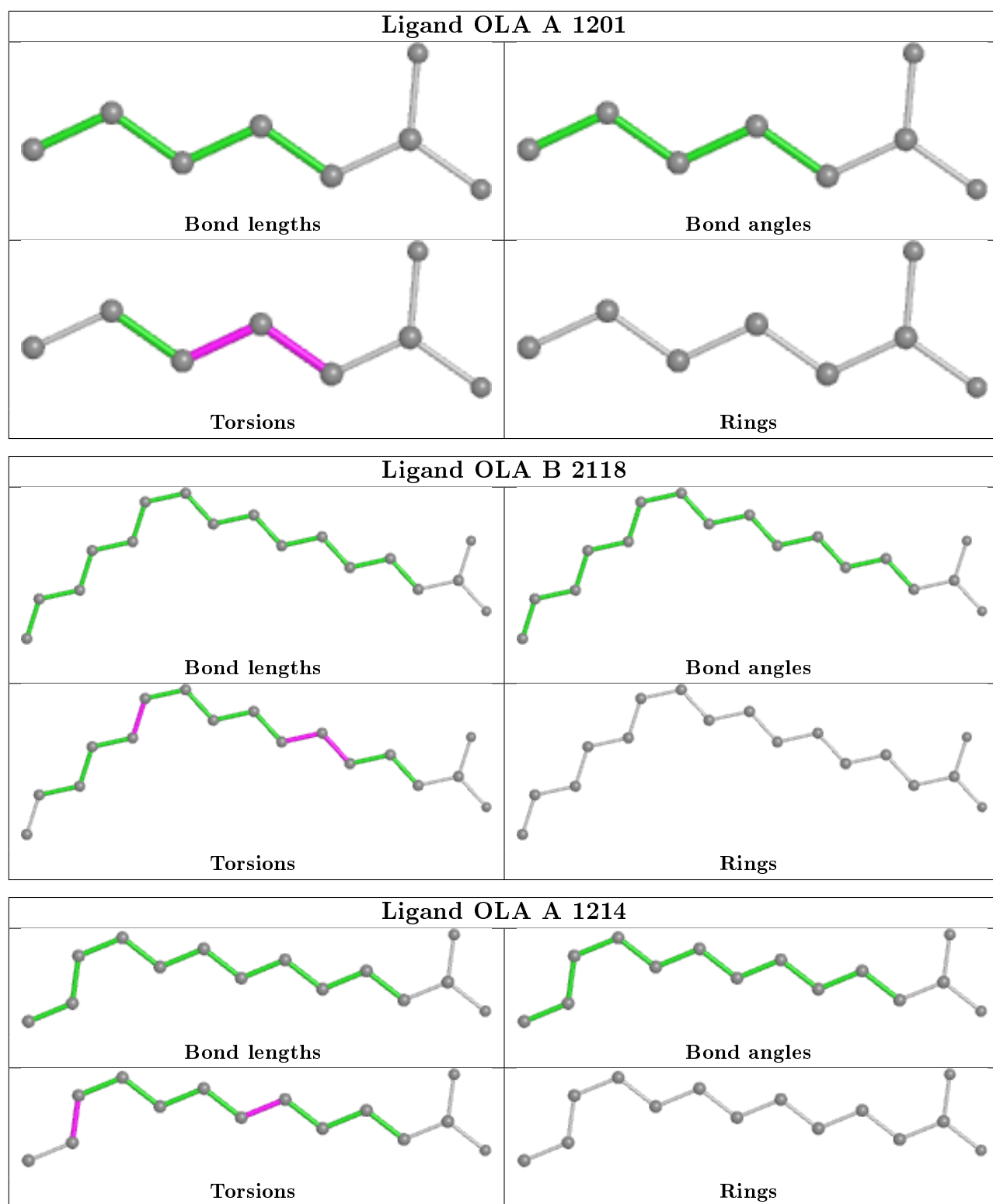
There are no ring outliers.

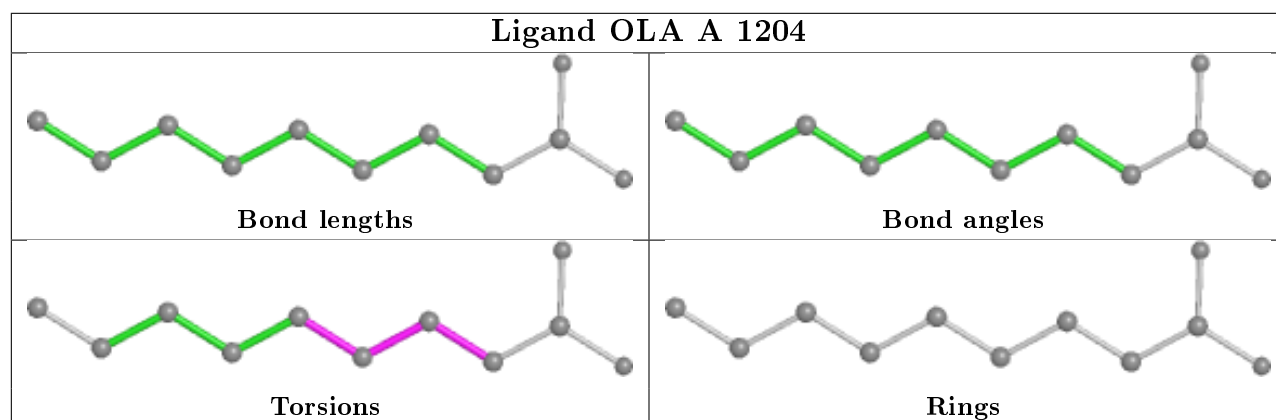
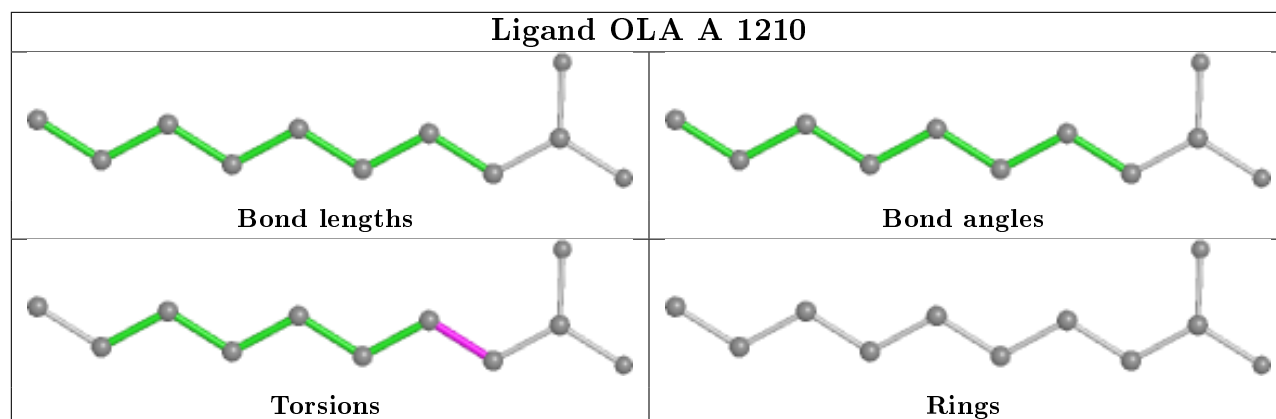
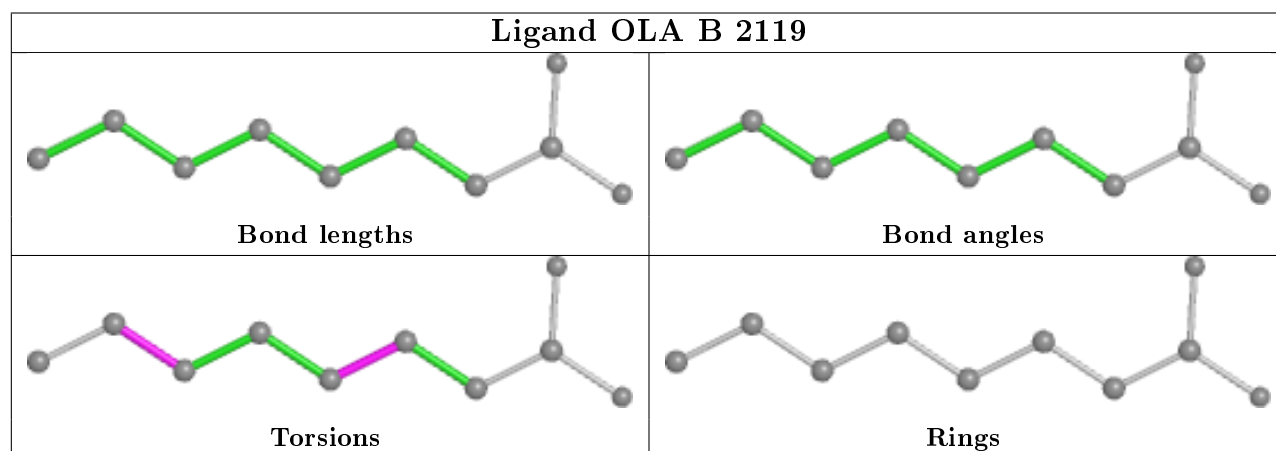
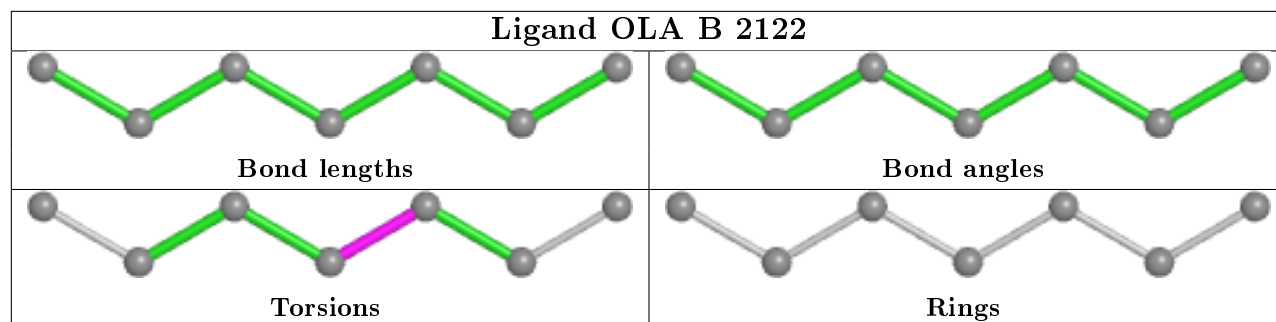
24 monomers are involved in 52 short contacts:

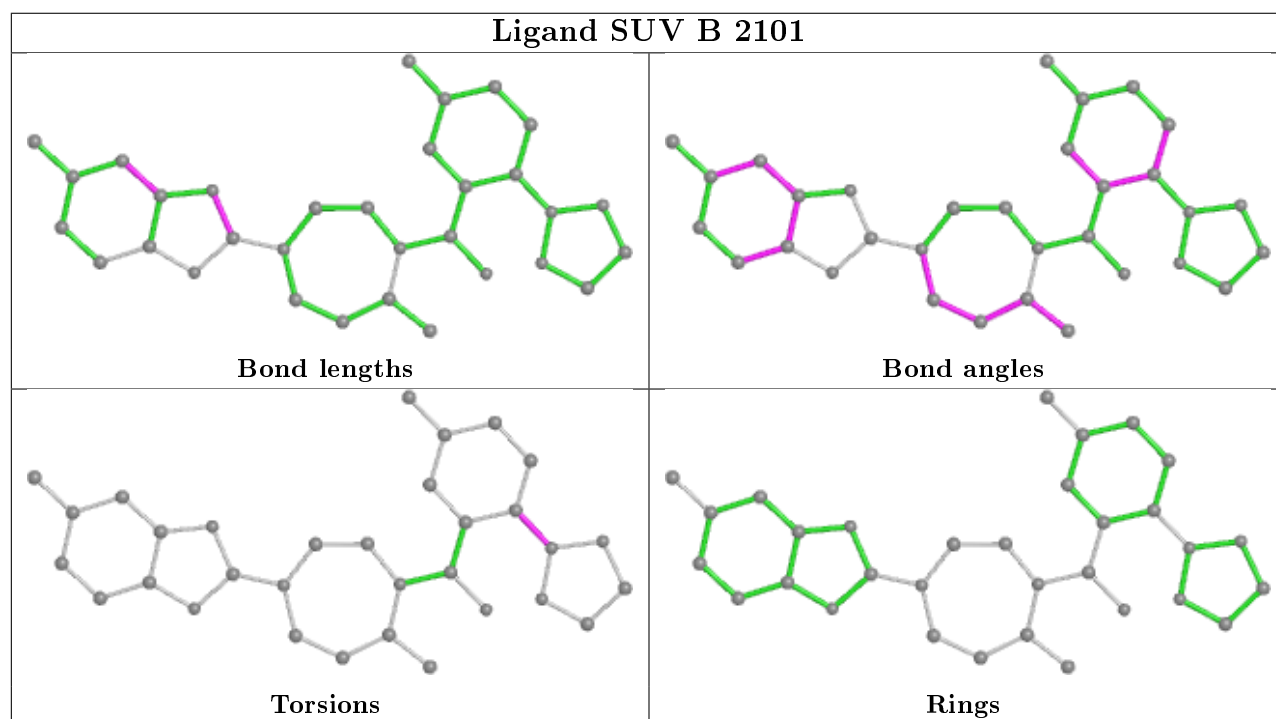
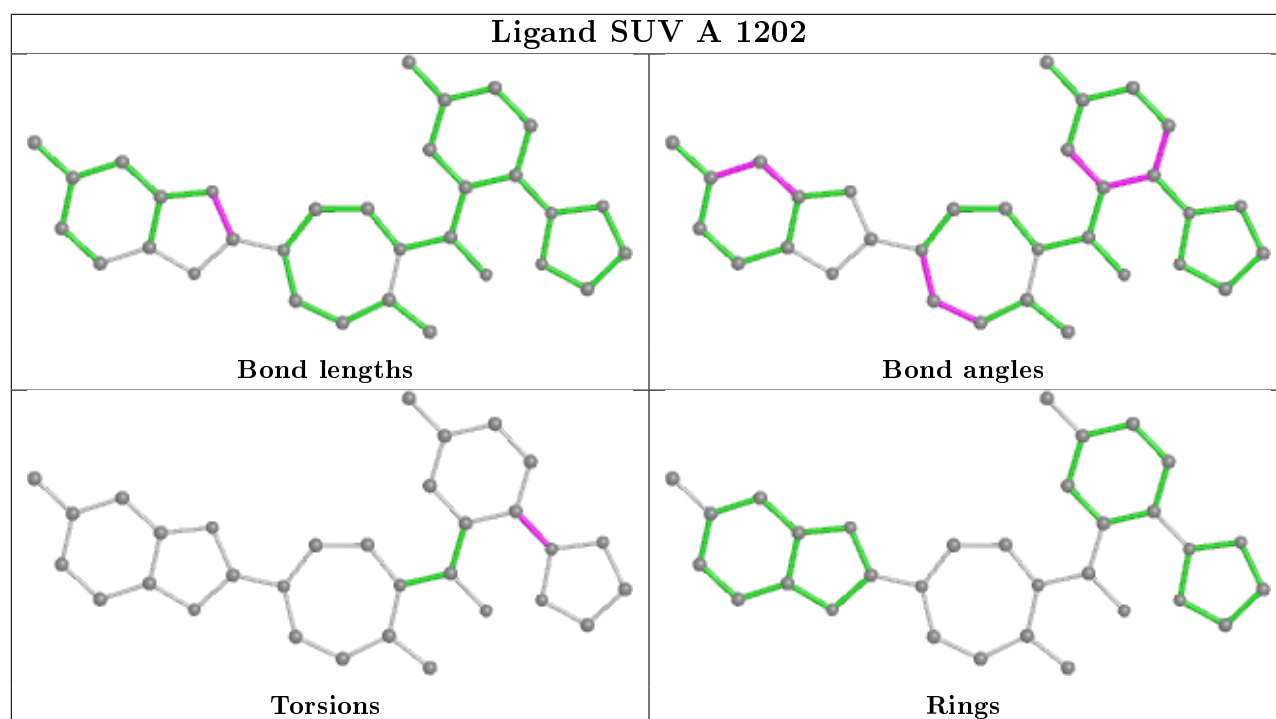
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1207	OLA	3	0
2	B	2121	OLA	2	0
2	A	1216	OLA	1	0
5	A	1217	PG4	2	0
5	B	2126	PG4	1	0
2	B	2116	OLA	1	0
2	A	1205	OLA	3	0
2	B	2117	OLA	1	0
2	B	2115	OLA	5	0
2	B	2118	OLA	2	0
2	A	1214	OLA	1	0
2	B	2122	OLA	3	0
2	B	2119	OLA	2	0
2	B	2105	OLA	2	0
2	A	1204	OLA	2	0
2	B	2109	OLA	1	0
3	A	1202	SUV	3	0
2	A	1209	OLA	2	0
3	B	2101	SUV	3	0
2	A	1213	OLA	6	0
2	B	2123	OLA	1	0
2	B	2113	OLA	3	0
2	B	2111	OLA	2	0
2	B	2106	OLA	1	0

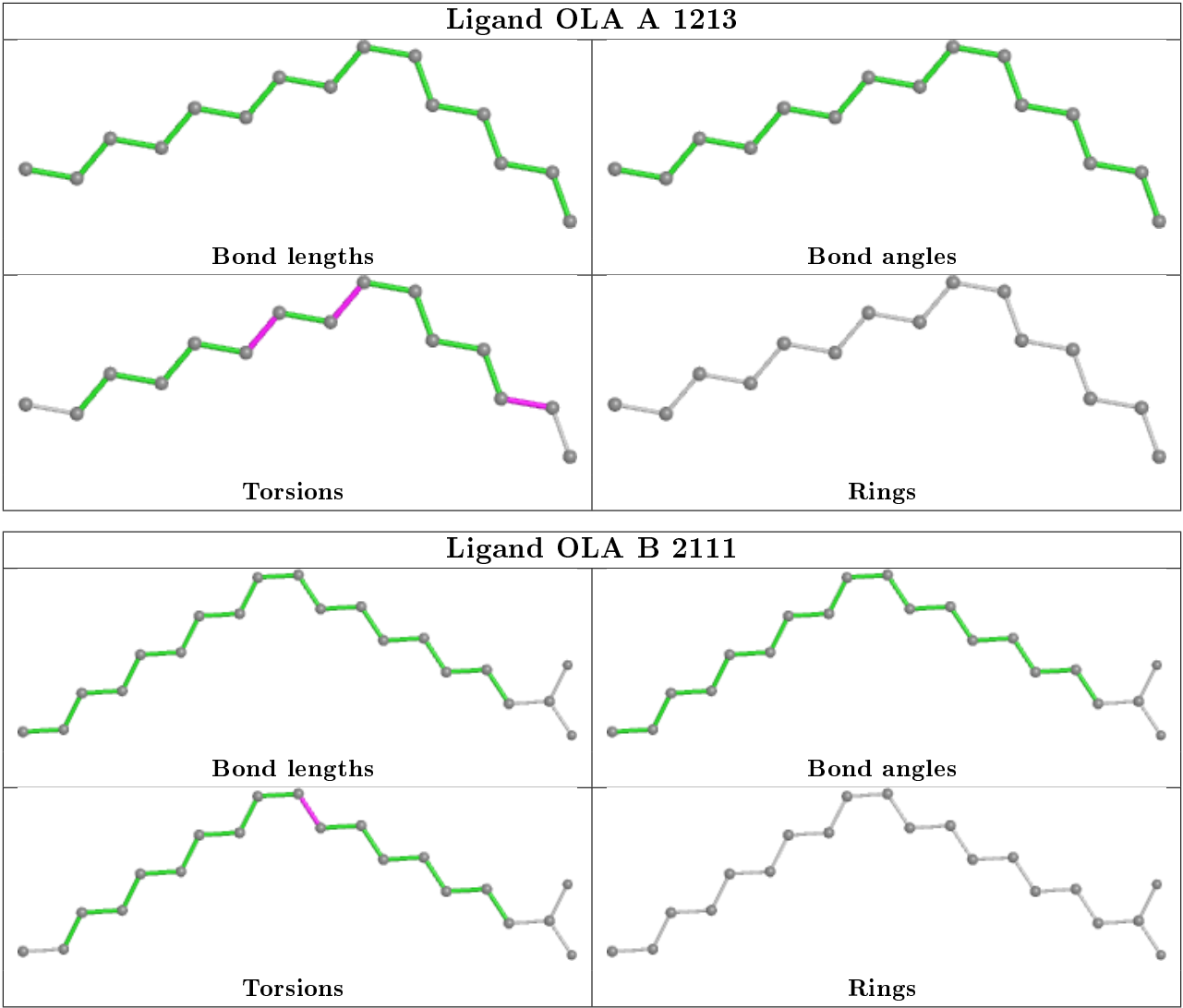
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	254:GLN	C	1001:GLY	N	2.90

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	498/564 (88%)	-0.53	1 (0%) 95 97	19, 36, 72, 120	0
1	B	500/564 (88%)	-0.52	2 (0%) 92 95	20, 36, 70, 108	0
All	All	998/1128 (88%)	-0.53	3 (0%) 94 96	19, 36, 72, 120	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	48	LEU	3.2
1	B	47	TYR	2.1
1	B	200	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	YCM	B	147	10/11	0.97	0.12	34,56,75,76	0
1	YCM	A	147	10/11	0.97	0.11	21,43,74,75	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

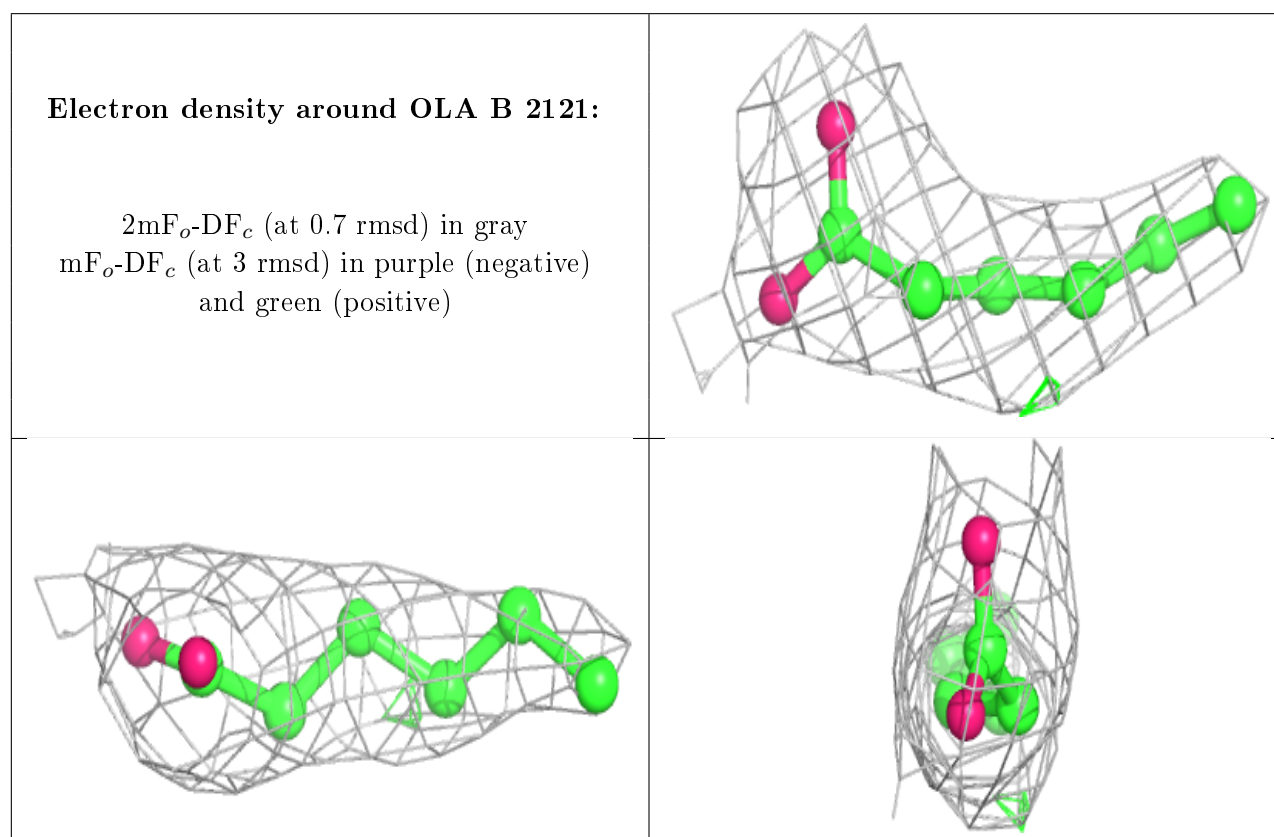
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	OLA	A	1212	7/20	0.86	0.29	59,62,68,68	0
2	OLA	B	2113	5/20	0.88	0.58	50,56,61,61	0
2	OLA	A	1208	9/20	0.89	0.14	54,68,82,82	0
2	OLA	B	2125	8/20	0.89	0.24	67,85,105,108	0
2	OLA	B	2108	9/20	0.89	0.21	59,64,78,80	0
2	OLA	A	1205	7/20	0.89	0.17	35,47,52,53	0
2	OLA	B	2114	7/20	0.89	0.31	71,81,95,97	0
4	NH4	B	2103	1/1	0.90	0.08	24,29,29,29	0
2	OLA	B	2121	8/20	0.91	0.20	58,60,66,69	0
5	PG4	A	1217	13/13	0.91	0.15	47,64,69,70	0
2	OLA	B	2124	5/20	0.91	0.30	35,41,52,52	0
2	OLA	B	2120	8/20	0.91	0.21	58,60,66,67	0
2	OLA	B	2112	7/20	0.91	0.29	46,53,59,60	0
2	OLA	B	2106	7/20	0.91	0.43	74,75,80,81	0
2	OLA	A	1204	11/20	0.92	0.36	53,60,76,77	0
2	OLA	B	2110	7/20	0.93	0.34	43,47,48,48	0
2	OLA	A	1210	11/20	0.93	0.18	44,58,64,64	0
2	OLA	B	2107	5/20	0.93	0.29	58,60,64,65	0
2	OLA	A	1209	8/20	0.94	0.29	54,55,60,62	0
2	OLA	B	2118	17/20	0.94	0.39	51,58,62,62	0
2	OLA	A	1214	14/20	0.94	0.24	43,63,77,77	0
5	PG4	B	2126	13/13	0.94	0.12	53,62,69,70	0
2	OLA	B	2111	20/20	0.94	0.26	23,53,75,76	0
2	OLA	B	2116	5/20	0.94	0.18	48,50,57,58	0
2	OLA	A	1207	6/20	0.94	0.21	47,56,59,59	0
4	NH4	B	2104	1/1	0.95	0.10	18,21,21,21	0
2	OLA	A	1201	8/20	0.95	0.15	24,44,53,57	0
2	OLA	A	1213	15/20	0.95	0.36	27,47,71,74	0
2	OLA	A	1216	6/20	0.95	0.23	20,31,32,34	0
2	OLA	B	2105	6/20	0.95	0.30	55,56,57,58	0
2	OLA	B	2122	7/20	0.95	0.29	36,48,52,52	0
2	OLA	B	2119	10/20	0.95	0.17	35,53,74,74	0
2	OLA	B	2117	7/20	0.95	0.28	35,45,50,52	0
2	OLA	B	2123	6/20	0.96	0.28	46,53,56,57	0
2	OLA	A	1211	6/20	0.96	0.22	34,36,43,44	0
2	OLA	B	2109	6/20	0.97	0.32	53,56,62,63	0
2	OLA	B	2115	4/20	0.97	0.48	56,57,57,58	0

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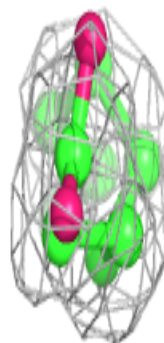
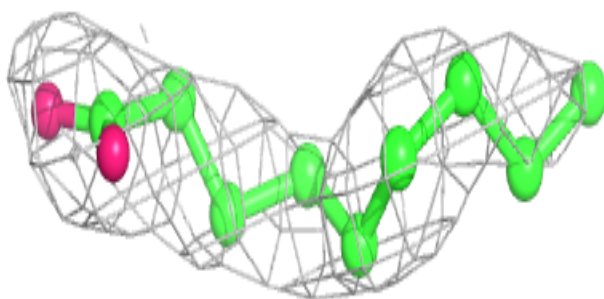
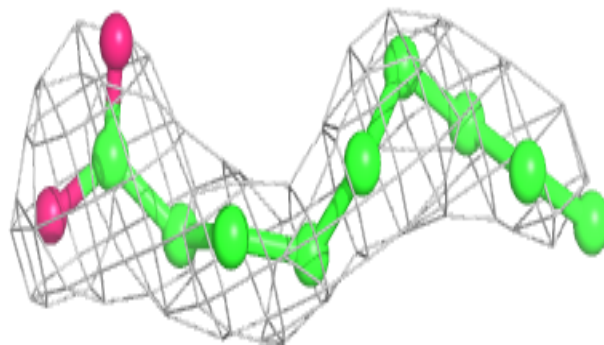
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SUV	A	1202	32/32	0.97	0.12	36,48,59,61	0
2	OLA	A	1215	6/20	0.97	0.17	60,62,67,72	0
4	NH4	B	2102	1/1	0.98	0.10	22,27,27,27	0
3	SUV	B	2101	32/32	0.98	0.12	38,47,57,62	0
4	NH4	A	1203	1/1	0.99	0.15	23,28,28,28	0
4	NH4	A	1206	1/1	0.99	0.07	24,29,29,29	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

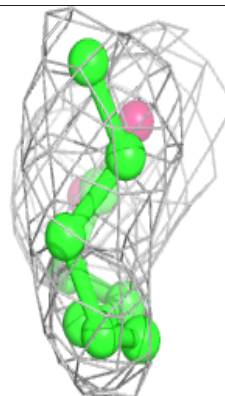
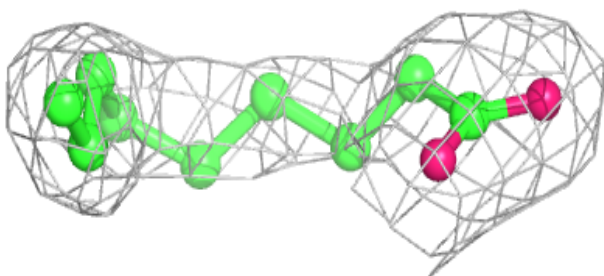
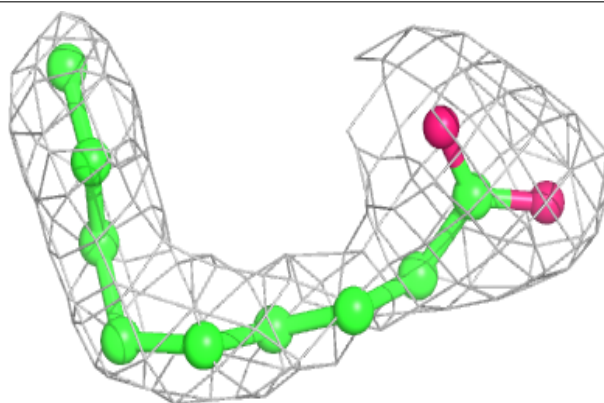


Electron density around OLA A 1204:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

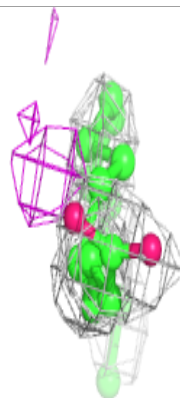
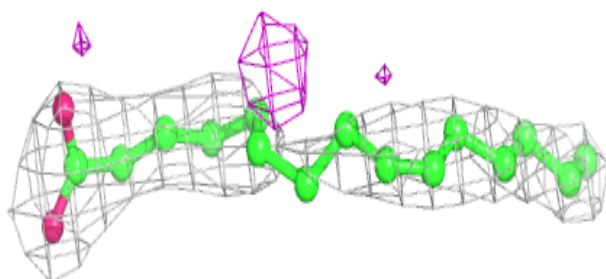
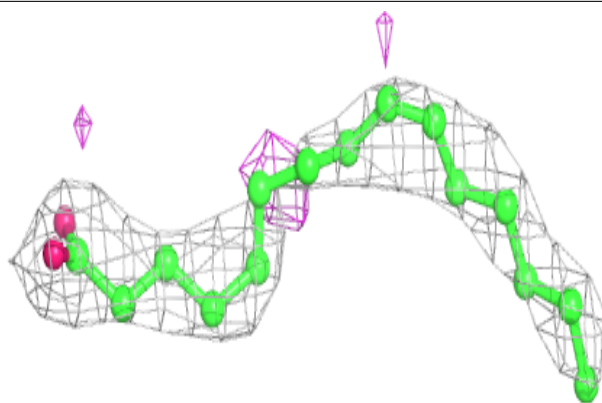
**Electron density around OLA A 1210:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

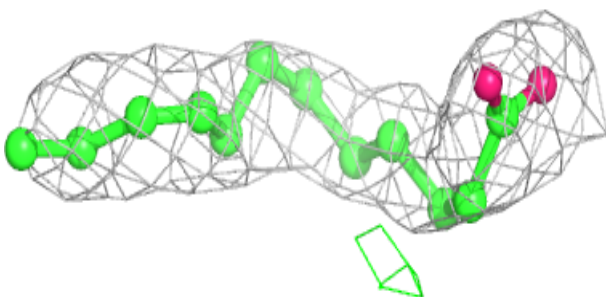
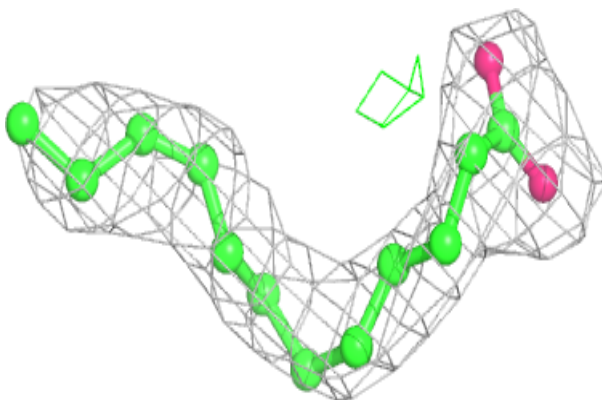


Electron density around OLA B 2118:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

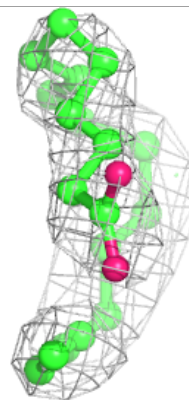
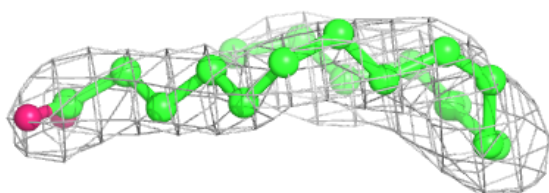
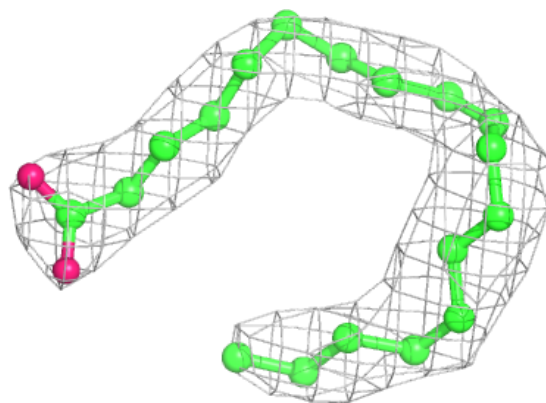
**Electron density around OLA A 1214:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

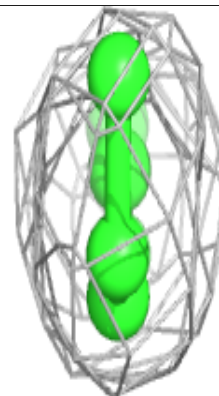
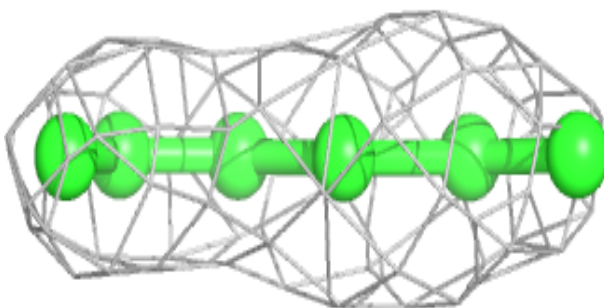
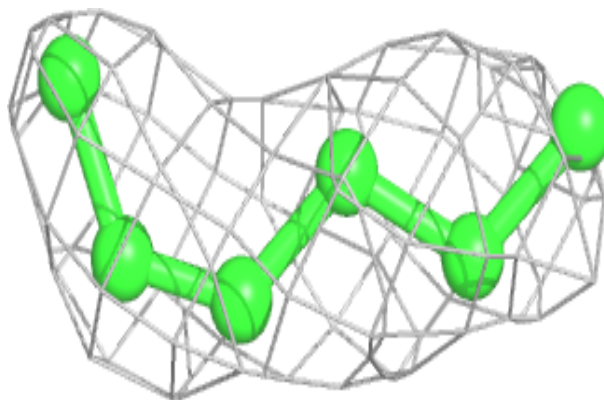


Electron density around OLA B 2111:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

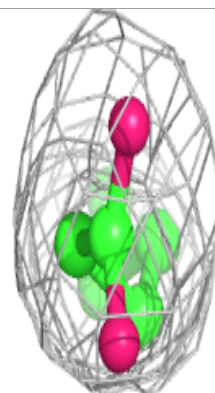
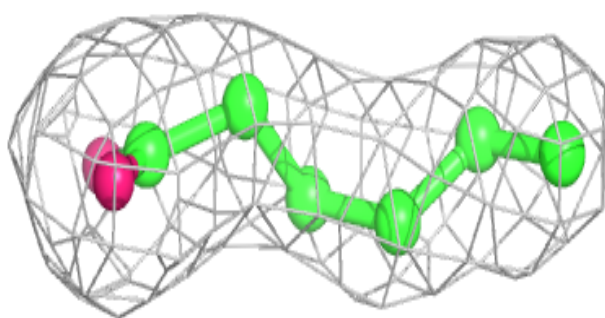
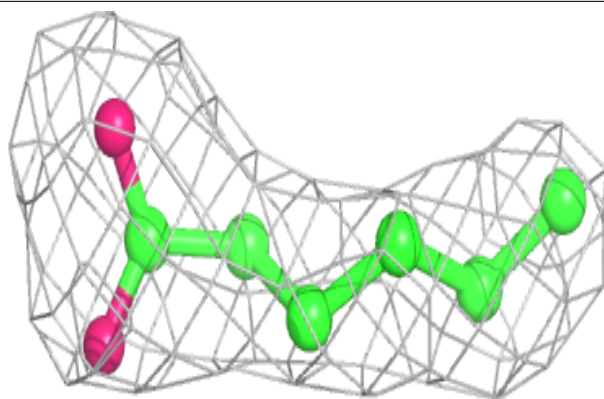
**Electron density around OLA A 1207:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

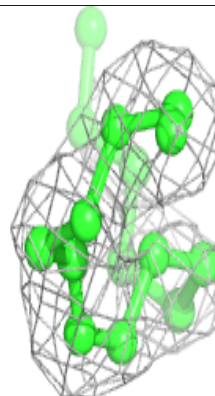
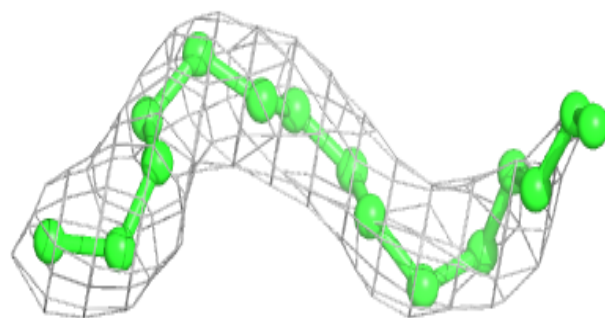
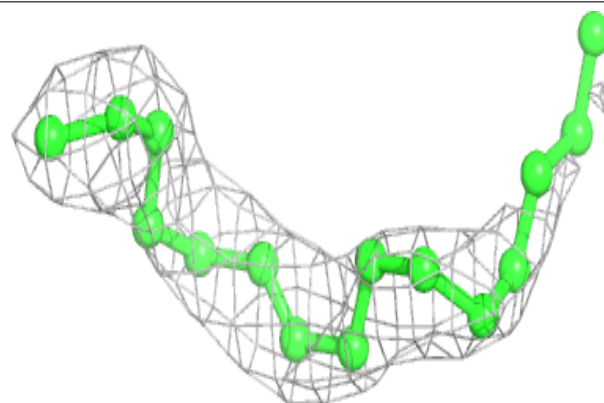


Electron density around OLA A 1201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

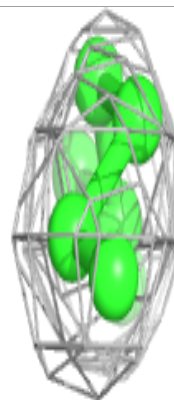
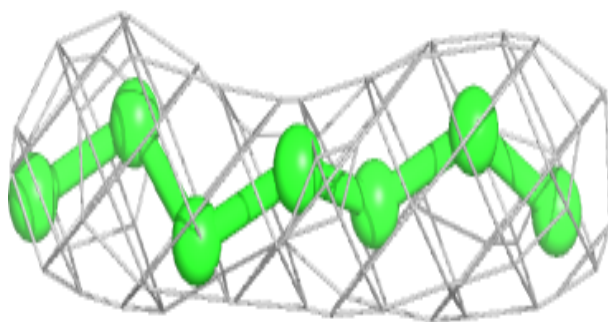
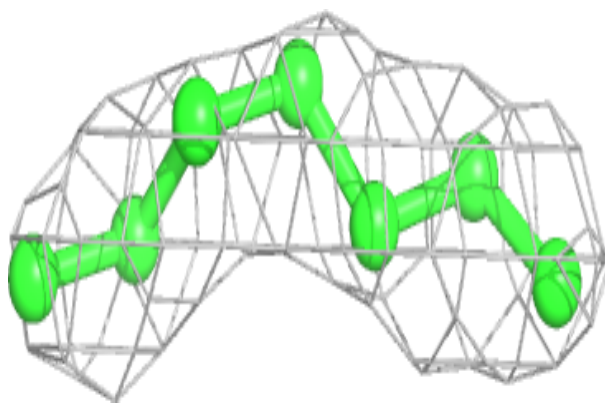
**Electron density around OLA A 1213:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

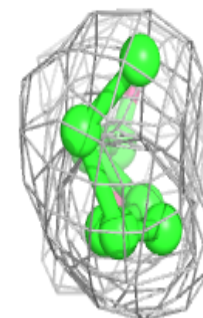
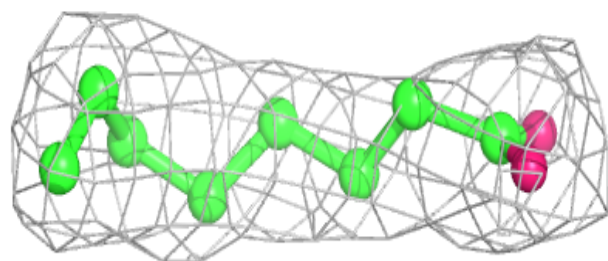
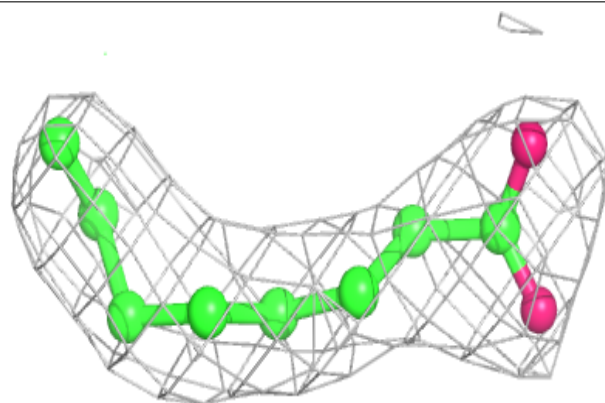


Electron density around OLA B 2122:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

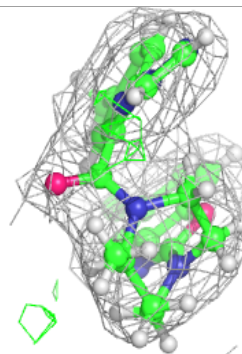
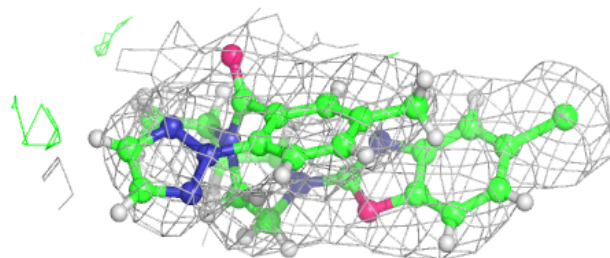
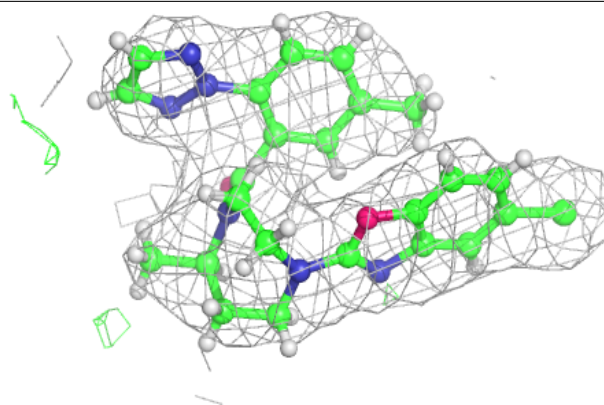
**Electron density around OLA B 2119:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

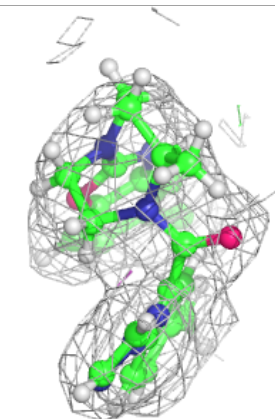
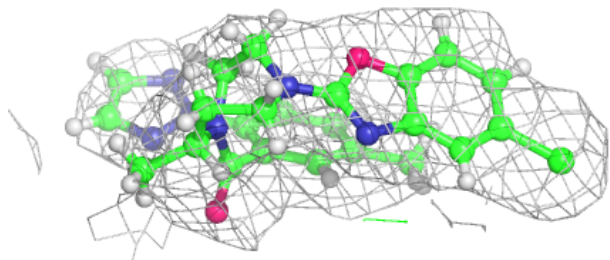
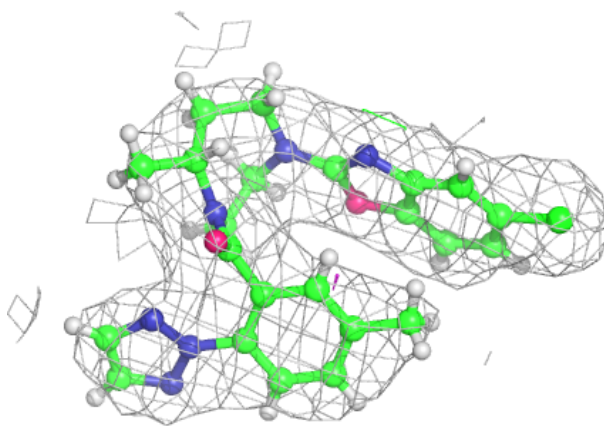


Electron density around SUV A 1202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around SUV B 2101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.